Effect of Interfacial Polymer Morphology on Solar Cell Performance

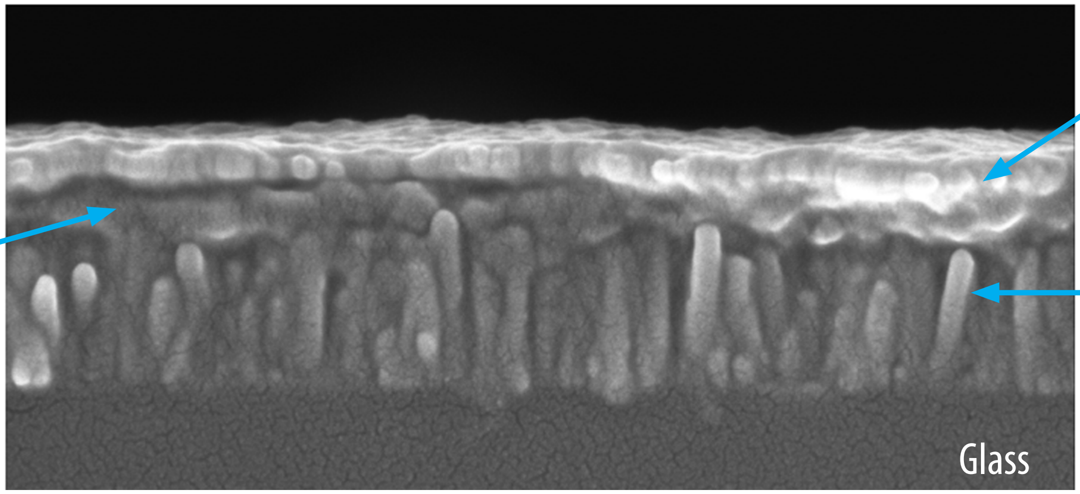

Figure 1: Cross-sectional scanning electron microscopy of a polythiophene-ZnO nanorod hybrid solar cell.

Organic-inorganic hybrid photovoltaics are studied by Sandia team

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The proliferation of new, high technology gadgets that make our life more convenient and enjoyable require evermore portable and reliable energy sources. Solar cells using organic photovoltaic (OPV) technology, with its light weight, flexibility, and inexpensive manufacturing process, appear to be uniquely suited to meet these new requirements. A subset of OPVs, called hybrid photovoltaics, uses organic polymers to generate carriers (electrons and holes) and inorganic metal oxide semiconductors as the electron acceptor material. The advantages of hybrid photovoltaics over purely organic counterparts include environmental stability, better electron transport, and the ability to optimize interfacial properties.

Sandia researchers, in collaboration with the National Renewable Energy Laboratory, have focused on understanding and optimizing hybrid solar cells that utilize nanostructured zinc oxide (ZnO) as the electron acceptor. The research challenges to making such solar cells practical are the ability to achieve highly dense oxide nanostructures (Figure 1), to infiltrate organic conjugated polymers into the ZnO nanostructures while maintaining polymer crystallinity, and to optimize the charge transfer process at the polymer-oxide heterojunctions. Synthesizing ZnO nanostructures from solution at low temperature is a particular expertise of the Sandia team. However, it was realized that the normally crystalline organic polythiophene forms a thin amorphous layer at the ZnO interface. This morphological change in the organic material is detrimental to solar cell performance as it shortens exciton diffusion length, reduces overlap with the solar spectrum, and degrades hole transport.

To understand and overcome this problem, Sandia modified the ZnO-polythiophene interface with a self-assembled monolayer of alkanethiols. These are long hydrocarbon chains that form chemical bonds with the ZnO but interact only weakly with the polythiophene. Since alkanethiols are also insulating molecules that form a barrier for electron transfer from polythiophene to ZnO, it was surprising when a higher than expected photocurrent was observed in these modified solar cells (Figure 2). Further research, using grazing-incidence X-ray diffraction (at the Stanford synchrotron) and femtosecond transient spectroscopy (at the Sandia-Los Alamos Center for Integrated Nanotechnologies in collaboration with Los Alamos National Laboratory), revealed that the alkanethiol layer indeed restored the crystallinity of the interfacial polymer (Figure 3). The crystalline form of the polymer greatly reduced the carrier recombination rate. Thus, despite the insulating alkanethiol layer between the polymer and the ZnO, the overall efficiency of the hybrid solar cell was improved.

These results highlight the importance of understanding nanometer-scale details of the interface, as nanoscale behavior has dramatic impact on the macroscopic performance of innovative new devices.

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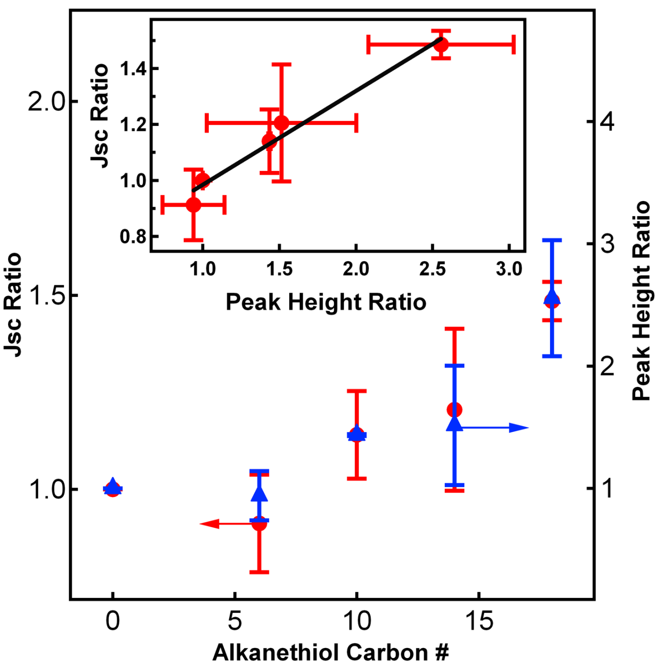

Figure 2: Increases in photocurrent (left axis, red circles) and polymer interchain order (right axis, blue triangles) as a function of the chain length of the interfacial organic modifier. Inset: the two increases are clearly correlated.

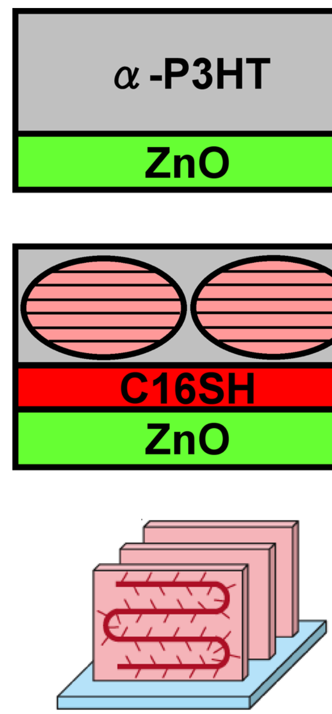

Figure 3: Schematics of polymer morphology change due to interfacial modification with a C_{16} alkane thiol at the ZnO interface. The amorphous polythiophene polymer(gray) becomes crystalline (pink areas) when the alkane thiol (red) is present. Detailed view of the crystalline regions (pink areas) is shown at bottom. (Y. Kim, et al. Nature Mater. 2006, 5, 197)

Sandia National Laboratories

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